

Furan. 2-ethynyl

Inchi: InChI=1S/C6H4O/c1-2-6-4-3-5-7-6/h1,3-5H
InchiKey: CTVCBOZMKFQEAP-UHFFFAOYSA-N
Formula: C6H4O
SMILES: C#Cc1ccco1
Mol. weight [g/mol]: 92.10

Physical Properties

| Property code | Value | Unit | Source |
|---------------|--------|--------|----------------|
| log10ws | -5.90 | | Crippen Method |
| logp | 1.261 | | Crippen Method |
| mcvol | 73.210 | ml/mol | McGowan Method |
| rinpola | 742.00 | | NIST Webbook |

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R511690&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpola: Non-polar retention indices

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